

C
event

Protein Modeling Event

1. Description

Students will use computer visualization and online resources to guide them in constructing physical models of proteins and in understanding how the structure of the protein determines the function. For 2012, students will model proteins involved in the regulation of apoptosis as they explore the discovery and treatment of a rare (one in a billion) genetic trait discovered through genome sequencing.

A TEAM OF UP TO: 3

IMPOUNT: Yes

APPROXIMATE TIME: 50 minutes for Part II & III

2. Event Parameters/Construction

Pre-build models will be impounded one hour before the competition begins.

- A. Students may bring up to five double-sided, 8.5"x11" pages of notes. Internet access is not permitted.
- B. Students must bring a writing instrument.
- C. Supervisors will provide all materials for on-site model construction.

3. The Competition

This event has three parts: a pre-build model, an on-site build model, & an exam.

Part I: The Pre-Build Model. Students will use a computer visualization program (Jmol; <http://cbm.msOE.edu/includes/jmol/SOJmols/2012PreBuild.html>) to design and construct a model of a specific protein based on atomic coordinate data, which can be accessed for free through the RCSB Protein Data Bank (<http://www.pdb.org>). For 2012, students will construct a model of caspase-3, based on chains A and B of the coordinate data found in the 1i3o.pdb file. Caspases are described in the August 2004 *RCSB Molecule of the Month* (<http://www.pdb.org/pdb/101/motm.do?momID=56>) by David S. Goodsell. The same constructed model of caspase-3 will be brought to all competitions; as the competition level increases, the scoring rubrics for the pre-build model will reflect higher expectations for model accuracy, detail and enhancements.

The final pre-build model must be based on the alpha carbon backbone display of the protein and must use a scale of 2 cm per amino acid. Students may use Mini-Toobers®, or other comparable material (e.g., Kwik Twists, 12 gauge dimensional house wire, etc.), to construct their pre-build model. Students will use materials of their own choosing to add functionally relevant features to their model (e.g. select amino acid sidechains, DNA or associated molecules). The additions to the model should focus on illustrating the significance of the structure to the function of the protein. A significant portion of the score will be derived from these additional features. Students must provide a 3"x5" note card explaining the additions to their model and what they represent. Students must deliver their pre-build model and 3"x5" card to judges at the competition site for impounding. Models must be picked up by the students after the competition.

Part II: The On-Site Model. During the on-site competition, students will design and build a physical model of a selected region of a protein using materials provided by the event supervisor. For the Invitational Competitions, students will model a selected region of Diablo (1g73.pdb). For Regional Competitions, students will model a selected region of XIAP (1i3o.pdb). For State Competitions, students will model a selected region of PARP (3od8.pdb). For the National Competition, students will model a selected region of MHC (1hsa.pdb), which is described in the February 2005 *RCSB Molecule of the Month* by David S. Goodsell (<http://www.rcsb.org/pdb/101/motm.do?momID=62>).

Students will utilize a computer provided with the Jmol application at the competition. Students must utilize only one of the identical computers provided at the competition with the above-mentioned files on it to guide their model construction. All construction materials for the model (Mini-Toobers^{®1}, foam amino acid sidechains, crosslinkers and plastic red and blue end caps) will be provided. Any model not handed to the judges by the end of the competition time will not be accepted for scoring.

Part III: The On-Site Written Exam. will be multiple choice/short answer questions about the relationship between protein structure and function, with an emphasis on apoptosis and bone marrow transplants.

Scoring

40% of the event score will be based on the pre-build protein model (Part I), 30% on the on-site build (Part II) and 30% on the written exam (Part III). The pre-build protein model (Part I) will be scored based on the accuracy and scale of the secondary structures, as well as the additions to the model (e.g. sidechains, DNA or associated molecules). Creative additions that do not support the molecular story will not receive full credit. The on-site build protein model (Part II) will be scored based on accuracy of folding the model and positioning specific amino acid sidechains. The exam (Part III) will be scored for accuracy. Ties will be broken using identified questions from the written exam.

Resources

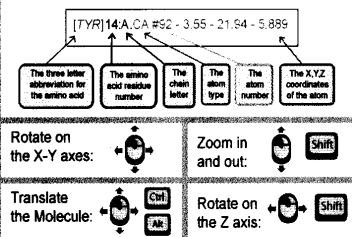
Event details and available kit information can be found at <http://cbm.msos.edu/stupro/so>.

MSOE CBM Science Olympiad Webpage (<http://cbm.msos.edu/stupro/so>) and the RCSB PDB Homepage (www.pdb.org) and website for the Science Olympiad (<http://education.pdb.org/olympiad>).

Mini-Toobers[®] are a product of 3D Molecular Designs, 1050 Market St, Suite CC130A Milwaukee, WI 53202, (414) 774-6562, Fax: (414) 774-3435, www.3dmoleculardesigns.com. Please visit this website to purchase your PreBuild materials.

Mouse Movements

Clicking on an atom provides information in the console window. This information is explained in detail below.



Display Formats

wireframe (displays stick bonds)
wireframe <value> (displays stick bonds with specific thickness)
example: wireframe 1.0

spacefill (displays atoms as spheres with atom radii equal to their Van der Waals radius)
example: spacefill

spacefill <value> (displays atoms as spheres with specific radius)
example: spacefill 1.25

backbone (displays alpha carbon backbone)
backbone <value> (displays backbone with specific thickness)
example: backbone 1.5

Exporting Images and Saving

To export a Jpeg file, click **File>Export>Export Image** from the top left of the display window.

An exported Jpeg file (.jpg) contains the information for both an image of your model as it appears in the display window at the time of exporting, as well as a record of your current state or progress.

To load your past progress using the saved information in an exported Jpeg file, drag the saved Jpeg file into the Jmol Display Window. This will automatically load your saved state or progress.

*Note: The Jpeg file must be located in the same folder as the PDB file that it uses in order to load correctly.

Method 1: color <selection type> <color name>
example: color background white

Method 2: color <selection type> [R,G,B]
example: color helix [15,255,110]

Method 3: select <selection type>
 color <color name or [R,G,B] code>
example: select hydrophobic
 color yellow

Default color mode: color CPK
 Color secondary structures: color structure

For a full list of the predefined colors available in Jmol, visit: <http://jmol.sourceforge.net/jscolors/>

Selection and Restriction

select <selection type> (selects part of the file)
example: select helix

restrict <selection type> (removes the display of everything except what was restricted)
example: restrict water

List of Common Selection Types:

backbone	sidechain	hydrophobic
hydrophilic	charged	hetero
water	nucleic	protein
helix	sheet	

*<letter> (for selecting by chain letter)

<number> (for selecting by residue number)

<number>-<number> (for selecting by residue range)

atomno=<number> (for selecting by atom number)

atomno=><number> and atomno<=<number> (for selecting by atom range)

<atom type> (for selecting by atom type)

Standard Sizes for SMART Team Models

backbone 1.5	hbond 1.0
wireframe 1.0	strut 1.0
spacefill 1.25	sbond 1.0

Bonds and Struts

Hydrogen Bonds:

calculate hbonds (adds hydrogen bonds to all selected areas)
 hbonds off (removes all hydrogen bonds in a selected area)
 hbonds <number> (displays hydrogen bonds with specific thickness)
 color hbonds <color> (colors hydrogen bonds)
 set hbondsSolid true (displays hydrogen bonds as solid lines)
 set hbondsSolid false (displays hydrogen bonds as dashed lines)
 set hbondsBackbone true (connects hydrogen bonds to the alpha carbon)
 set hbondsBackbone false (connects hydrogen bonds to the nitrogen and oxygen atoms)

To add or remove a single hbond, select only the two amino acids that the hbond connects and use the hbonds 1.0 or hbonds off command

example: select 716 or 1341 *example:* select 14 or 342
 hbonds 1.0 hbonds off

Disulfide Bonds:

ssbonds on (adds disulfide bonds to all selected areas)
 ssbonds off (removes disulfide bonds)
 ssbonds <number> (displays with specific thickness)
 color ssbonds <color> (colors disulfide bonds)
 set ssbonds backbone (connects disulfide bonds to the alpha carbon)
 set ssbonds sidechain (connects disulfide bonds to the nitrogen and oxygen atoms)

To add or remove a single ssbond, select only the two amino acids that the ssbond connects and use the ssbonds 1.0 or ssbonds off command

example: select 716 or 1341 *example:* select 14 or 342
 ssbonds 1.0 ssbonds off

Struts:

calculate struts (adds structural supports called struts to all selected protein areas)
 struts off (removes struts)
 struts <number> (displays with specific thickness)
 color struts <color> (colors struts)

To add or remove a single strut, select only the two atoms that the strut connects and use the strut or strut off command

example: select atomno=716 or atomno=1341 *example:* select atomno=14 or atomno=342
 connect strut connect strut delete
 strut 1.0

Adding a "Clean" Sidechain:

To select and display only the atoms of the sidechain of a specific amino acid, you want to use the select command followed by the amino acid name/number and end with the and (sidechain or alpha) text.

```
select cys30 and (sidechain or alpha)
spacefill 1.25
wireframe 1.0
```

To remove an incorrectly displayed sidechain:

```
select cys30
spacefill off
wireframe off
```

Additional Resources:

General Protein Structure:
<http://cbm.msoe.edu/stupro/so/ProteinStructure.html>

Official Jmol Command Database:
<http://jmol.sourceforge.net>

CBM Jmol Training Guide E-book
<http://cbm.msoe.edu/teachRes/jmol/trainingguide/>

RSCB Protein Data Bank
<http://www.pdb.org>

Jmol Wiki Page
<http://wiki.jmol.org/index.php/>